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This presentation discusses the construction of the new software framework that supports, pluggable multi-physics, hybrid parallelism for HPC, and productive work flows, to deliver analyzed results by using high-fidelity solutions of hyperbolic conservation laws. The new software framework is called SOLVer CONstructor, i.e., SOLVCON; it is a platform to construct PDE-solving codes.

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SOLVCON: An Unstructured PDE Framework

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October 2011

New Software Framework for Solving Hyperbolic Conservation Laws

- This presentation discusses the construction of the new software framework that supports
  - pluggable multi-physics,
  - hybrid parallelism for HPC, and
  - productive work flows,

  to deliver analyzed results by using high-fidelity solutions of hyperbolic conservation laws.
- The new software framework is called SOLVer CONStructor, i.e., SOLVCON; it is a platform to construct PDE-solving codes.

Outline

1. SOLVCON Framework
   - Design of the Software Framework
   - Code Development for SOLVCON

Python Programming Language

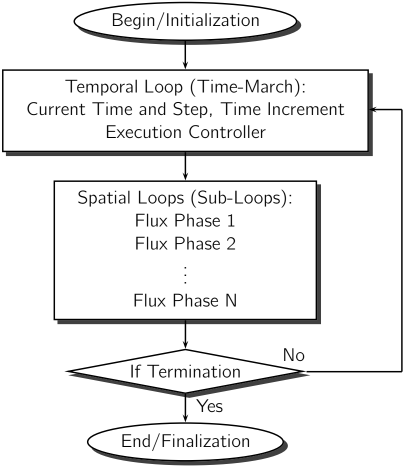
- Python enables high-level constructs:
  - Pluggable multi-physics.
  - Automatic hybrid parallelism.
  - Parallel I/O and in situ analysis/visualization.
- Python is a dynamically-typed programming language.
  - Support multiple programming paradigms: procedural (like Fortran or C), object-oriented (like C++ or Java), and functional (like Lisp or Scheme).
  - Realize high-level construct: type registries, plug-ins, etc.
- Python is designed to glue multiple programming languages together.
  - Use CUDA, C, pthread, and MPI simultaneously.
- Python is suitable to extend SOLVCON's functionalities:
  - 100+ packages in standard library and 13000+ 3rd-party packages.
  - Wrappers to many existing toolkits: VTK, netCDF, MPI, etc.

Python and C/C++

- Python and C - Ctypes
  - Compile the C code as a shared object
  - Python/ctypes cannot read in c header files so some of the contents of the header files will need to be rewritten in python, function definitions do not need to be rewritten.
  - Load the library from python using ctypes module and save to an object
  - This object contains each subroutine from the shared object file.
- Python and C++ - Boost
  - This is accomplished by writing wrappers to the C++ classes
  - Does not require any changes to the C++ code
  - I have not used this before as python handles the objects

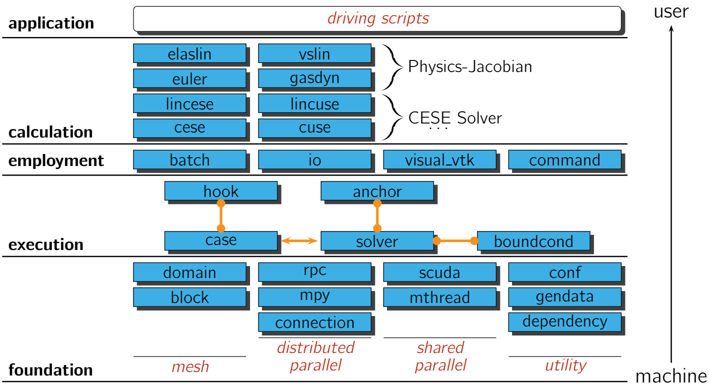
Two-Loop Structure

- All time-accurate finite-volume methods contain two loops.
  - Temporal loop time-marches for temporal integration.
  - Spatial loops iterate over elements to calculate flux.
- These two loops form the basic structure of SOLVCON.



Five-Layer Architecture

- Code is organized by using Python modules (blue solid boxes).
- A module depends only on other modules in the same layer or in the lower layers.
- The two-loop structure is hosted in the execution layer.



Driving Scripts

- The driving scripts are the highest-level construct of SOLVCON.
- A driving script must create a `Case` object and call its (i) `init()`, (ii) `run()`, and (iii) `cleanup()` methods.
    - The `Case` object represents the overall execution flow of the simulation, and contains the temporal loop.
- The driving scripts can specify logic to the simulations in addition to parameters.
    - Anything higher than the foundation layer (the lowest layer) can be replaced by code written in driving scripts.
    - Including but not limited to `Case`, `Solver`, `BC` classes, `Hook` and `Anchor` classes.
- SOLVCON does not use input files, but uses driving scripts instead (because Python code needs no explicit compilation).

Calculation

- Solver
  - This is a generic hyperbolic non-linear solver that has been optimized for both CPU and GPU and has been simplified for linear equations.
  - This is accomplished through the use of pre-processors that optimize/simplified certain portions of the code
  - Through the use of functional pointers these routines will call the required Jacobian subroutines.
- Constitutive Equations
  - These subroutines are called by the solver schemes and calculate the Jacobian and fluxes
  - SOLVCON has built in support for Euler and linear solvers.
  - New physics can be added by creating new Jacobian routines and by modifying certain parts of the default case and solver codes.
  - This is accomplished through inheritance

Employment

- batch: Used to submit parallel jobs on a cluster. Built in support for Torque
- io: Reads in the mesh and writes the VTK output files
  - Input capable of reading in: Gambit Neutral and Genesis/Exodus.
  - Output capable of writing: VTK in both serial and parallel, ASCII and binary.
- visual_vtk: Provides real time visualization and access to VTK through the VTK python wrappers.
- command: Provides the infrastructure for command line arguments

Execution

- hook: Allocates locations where the user can insert code into the temporal loop. Code inserted here can run in serial mode only
- anchor: Similar to the hook but the code is inserted into spatial loop. Code inserted here runs on each compute node.
- case: Provides the basic helper subroutines to support the solver such as:
  - cfl calculations
  - Convergence checks
  - I/O post processing support such as track results along a line or at a particular point
- solver: Defines the structure of the main program.
  - Defines the main data structure
  - Initializes/creates the data in the structure
  - Provides the routine to be called in the marching routine

Boundary-Condition Treatments

- SOLVCON uses ghost cells to treat boundary conditions (BC).
  - BC treatments depend on (i) numerical algorithms, (i) physical models, and (iii) mesh data structures.
- SOLVCON decouples BC treatments from numerical algorithms.
  - The `BC` class hierarchy is used to hold the code.
- A BC treatment is a spatial sub-loop that iterates over only boundary cells.

```
ConcreteSolver(Solver):
  def bound_flux():
    for bc in self.bclist:
      bc.bound_flux()
  def bound_gradient():
    for bc in self.bclist:
      bc.bound_gradient()
```

```
ConcreteBC(BC):


  def bound_flux():
    ...

  def bound_gradient():
    ...
```

Boundary-Conditions

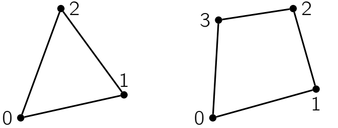
- Boundary conditions can be defined by either the solver or the physics.
- Boundary conditions specified by the solver are generic and are applicable to all physics. These boundary conditions are:
  - Non-reflecting
  - Periodic
- Boundary conditions specified by the physics are only available to the physics that creates them. Some examples are:
  - Non-Viscous wall
  - Pressure inlet/outlet
  - Non-Conducting
  - ...

Foundation

- Mesh
  - domain: oversees the domain decomposition using Metis or Scotch and distributes the domains over the network
  - block: Provides the data structures for the unstructured mesh
- distributed parallel
  - rpc: Remote Procedure call and inter-process communication
  - mpy: Python wrappers to MPI
  - connection: Remote connections and communications between nodes
- Shared parallel
  - scuda: A wrapper to the CUDA shared libraries through ctypes
  - mthread: Multi-threading though pthreads, OpenMP, MPI
- utility
  - conf: Info about the configuration of SOLVCON
  - gendata: Generic data structure
  - dependency: Manages the external shared libraries

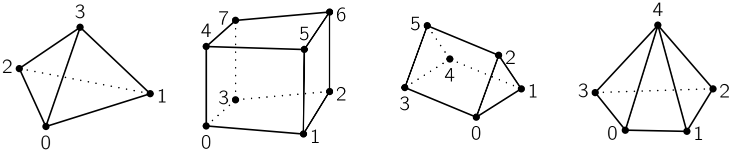
Currently Supported 2/3D Primitive shapes

- Two-dimensional elements:



triangle quadrilateral

- Three-dimensional elements:



tetrahedron hexahedron prism pyramid

Data Structures of Unstructured Meshes

- Three types of entities: nodes, faces, and cells.
- The spatial domain of interest is covered by non-overlapping cells.
- Two sets of arrays define the meshes.

Connectivity

- `clnds`: nodes in each cell.
- `clfcs`: faces in each cell.
- `fcnds`: nodes in each face.
- `fccls`: cells related by each face.

Geometry

- `ndcrd`: coordinates of each node.
- `fccnd`: center of each face.
- `fcnml`: unit normal vector of each face.
- `fcara`: area of each face.
- `clcnd`: center of each cell.
- `clvol`: volume of each cell.

On-the-Fly Analysis

- Solution processing is not part of the numerical algorithms.
- SOLVCON uses the callback mechanism to separate the supportive functionalities from numerical algorithms and physical models.
  - `Hook`: The outer temporal loop.
  - `Anchor`: The inner spatial loops.
- Example 1: Initial condition.
  - SOLVCON calls the `preloop()` method before entering the temporal loop.
- Example 2: Calculate physical quantities.
  - SOLVCON calls the `postmarch()` method after finishing all spatial loops for each time step.
- The analysis code can be packaged with solver kernels.

Coding for In Situ Visualization

- SOLVCON directly calls external visualizing libraries by using Python.
  - Currently support VTK.
- VTK interface is provided in SOLVCON.
  - Provide one-way data converter from SOLVCON to VTK.
  - Use VTK's official Python wrappers to access all VTK functionalities, e.g., cut surface, contour, iso-surface, etc.
- In situ visualization is programmed in driving scripts.
  - Visualization differs from one case to another.
  - No hard-wired code.
- The driving scripts become an application program that can deliver analyzed results including graphic files.

SOLVCON is Open-Sourced

- Released under GNU GPL v2 with full source.
  - Freely available at `http://solvcon.net/`
- Systematic open-source practices: (i) Distributed version control system, (ii) unit testing, (iii) issue tracking, (iv) continuous integration, (v) auto-generated API documentation.